

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020123\
 Data File : BF132252.D
 Acq On : 01 Feb 2023 10:40
 Operator : CG\JU
 Sample : PB150575BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB150575BL

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132252.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.313	415	421	430	rBV	1349582	1760125	31.45%	4.896%
2	5.696	480	486	489	rBV	4079236	4231769	75.61%	11.770%
3	6.684	648	654	657	rBV	3672993	4208945	75.20%	11.707%
4	7.066	716	719	723	rVB	1231198	998791	17.84%	2.778%
5	7.631	810	815	818	rBV	2931396	2866622	51.22%	7.973%
6	8.354	934	938	941	rBV	1758925	1354251	24.20%	3.767%
7	9.437	1117	1122	1125	rBV	5537612	5282096	94.37%	14.692%
8	10.119	1235	1238	1242	rVB	1937420	1550748	27.71%	4.313%
9	10.913	1369	1373	1376	rBV	3853784	3408002	60.89%	9.479%
10	11.619	1489	1493	1496	rBV	1883720	1601454	28.61%	4.454%
11	13.013	1727	1730	1734	rBV	157643	133337	2.38%	0.371%
12	13.213	1759	1764	1767	rBV	5663729	5597177	100.00%	15.568%
13	13.724	1848	1851	1855	rBV	179012	144928	2.59%	0.403%
14	14.277	1941	1945	1949	rBV	1502373	1324639	23.67%	3.684%
15	15.866	2209	2215	2225	rBV	935309	1211554	21.65%	3.370%
16	18.424	2639	2650	2666	rVB4	58180	278262	4.97%	0.774%

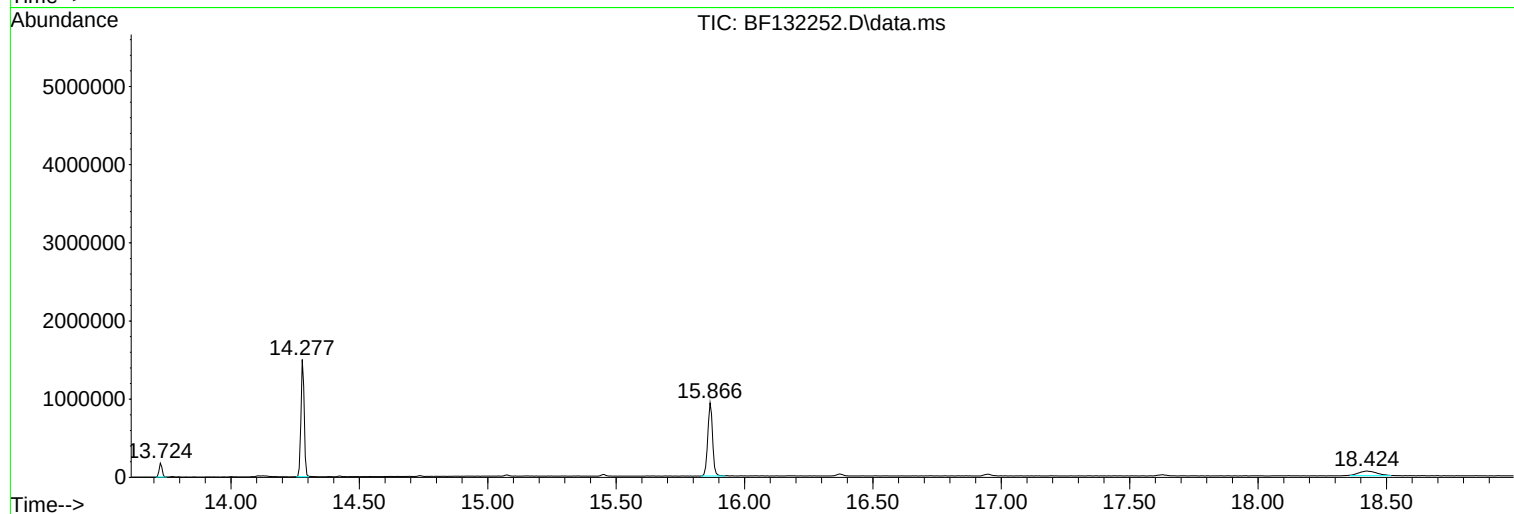
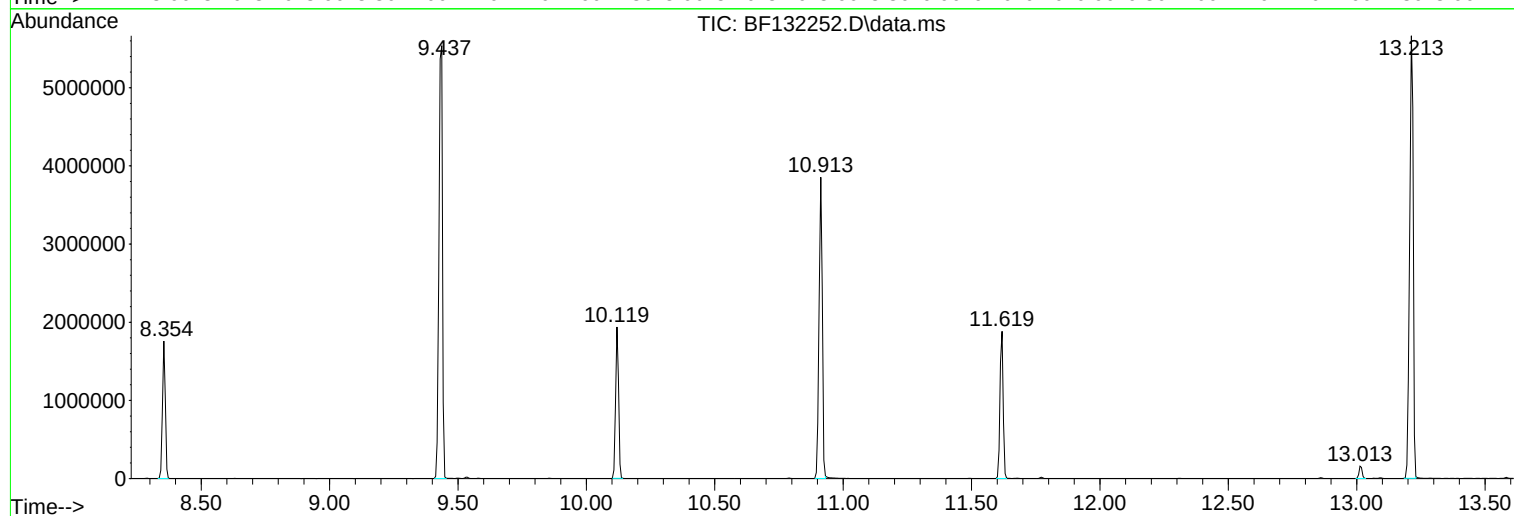
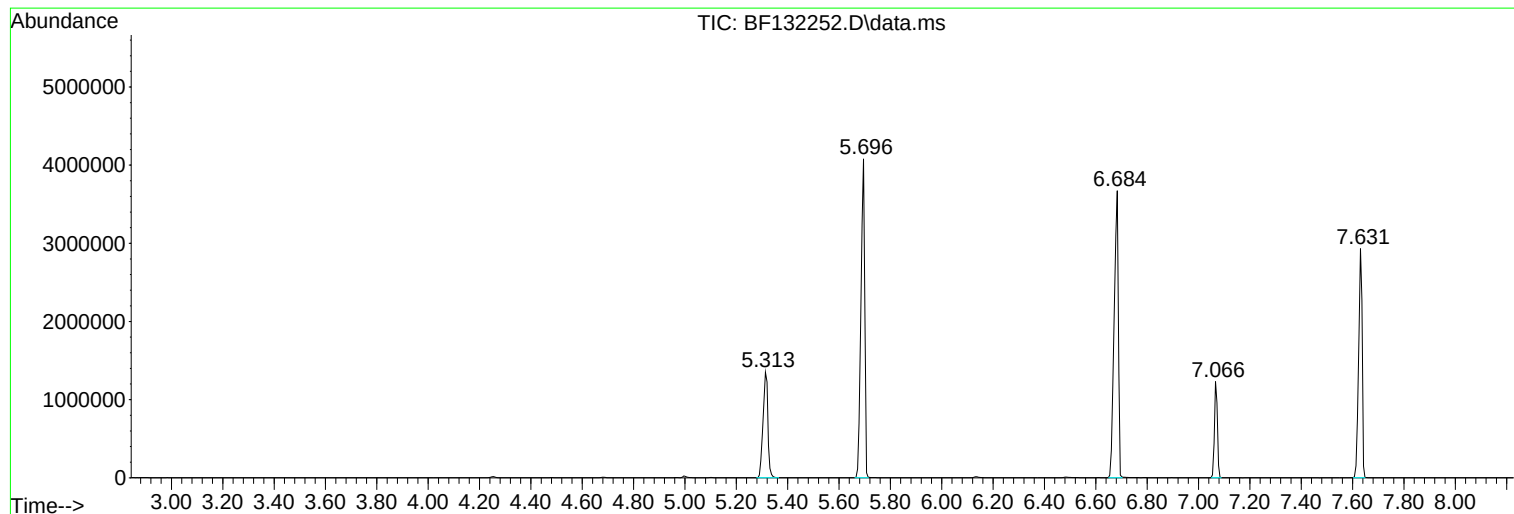
Sum of corrected areas: 35952700

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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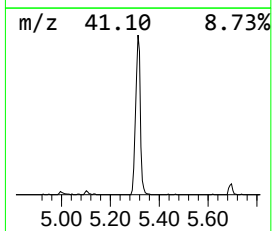
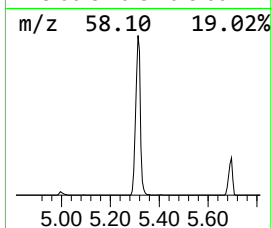
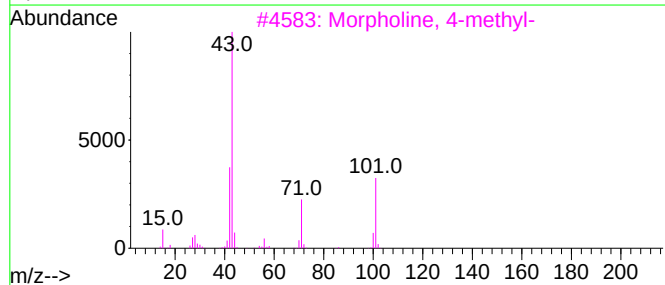
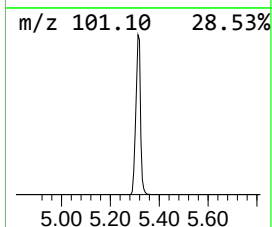
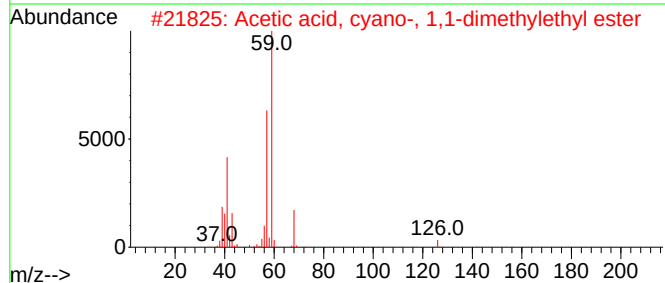
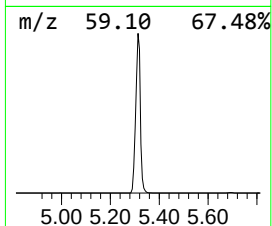
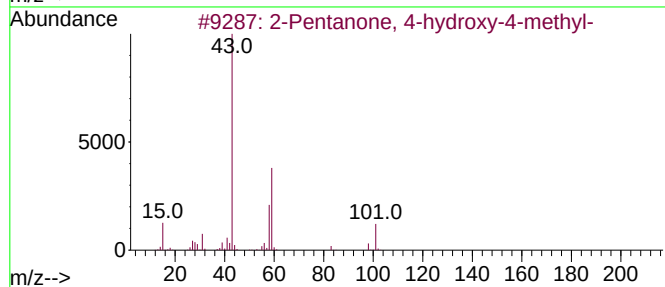
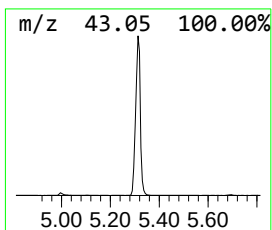
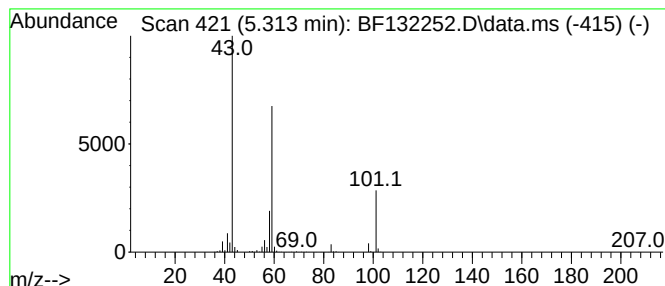
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.313	35.25 ng	1760130	1,4-Dichlorobenzene-d4			7.066
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9
4	Acetone		58	C3H6O	000067-64-1	9
5	Guanidine		59	CH5N3	000113-00-8	9



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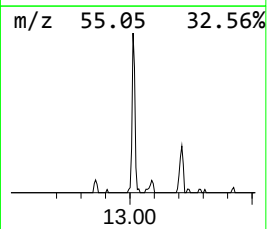
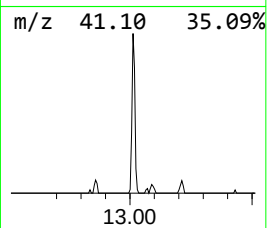
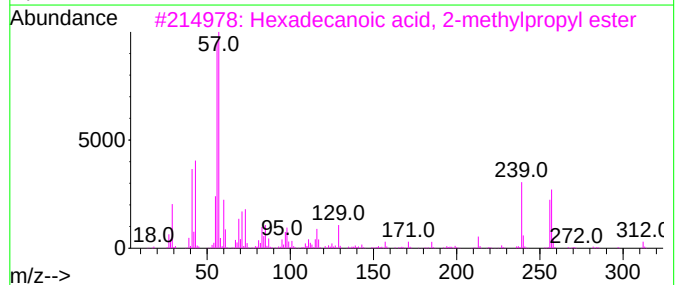
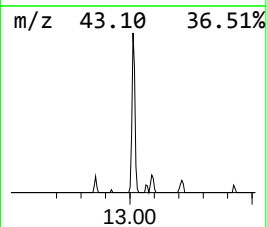
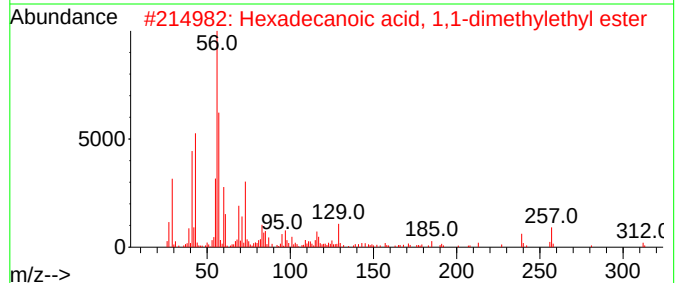
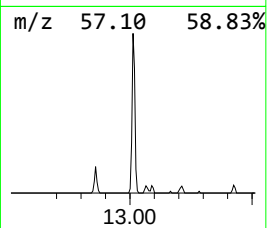
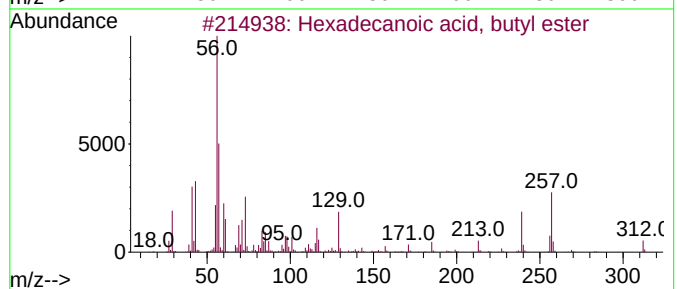
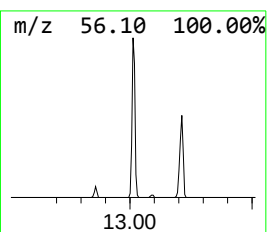
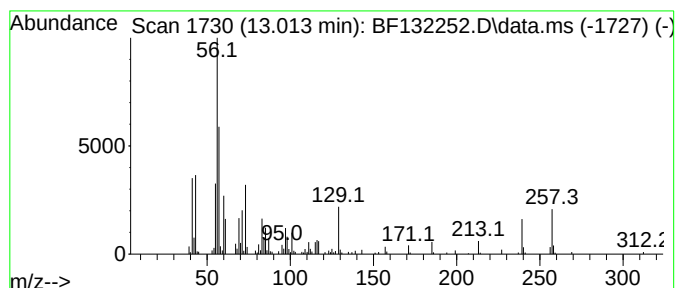
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.013	2.01 ng	133337	Chrysene-d12	14.277	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	96
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	72
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	43
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35



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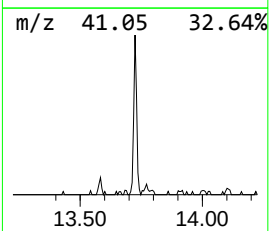
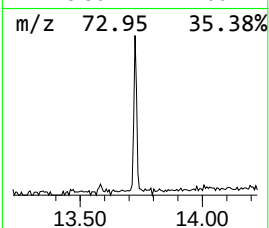
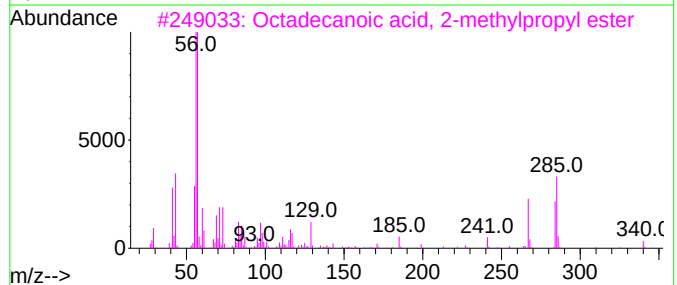
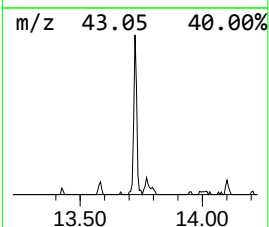
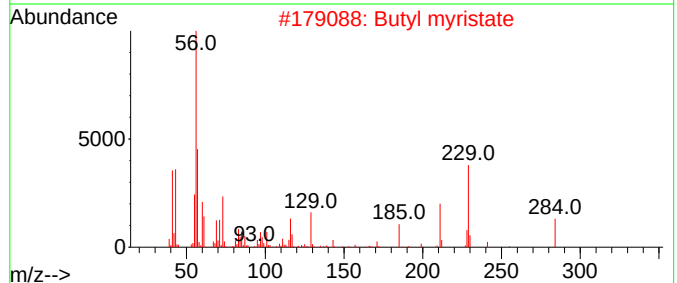
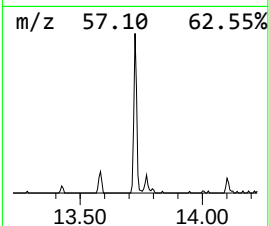
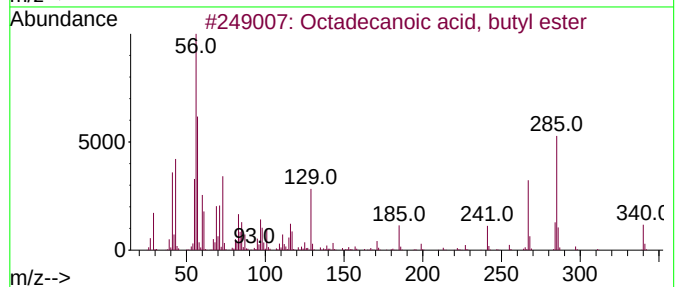
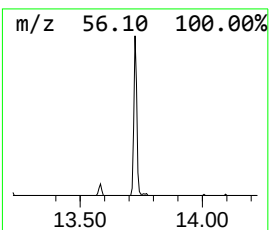
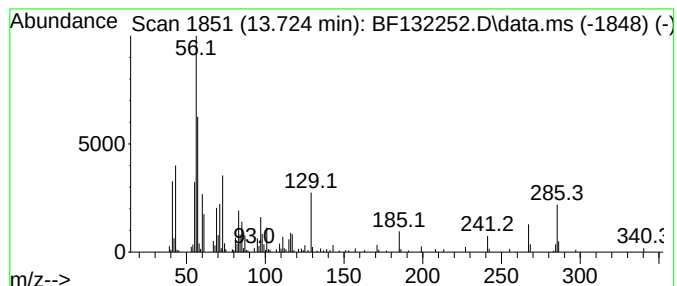
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Peak Number 3 Octadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.725	2.19 ng	144928	Chrysene-d12	14.277	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2	Butyl myristate	284	C18H36O2	000110-36-1	53
3	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	49
4	Nipecotic acid	129	C6H11NO2	000498-95-3	47
5	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	32



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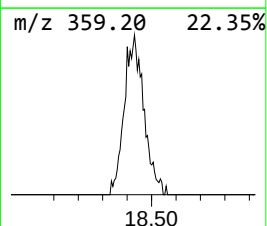
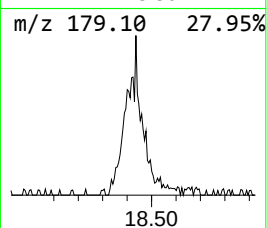
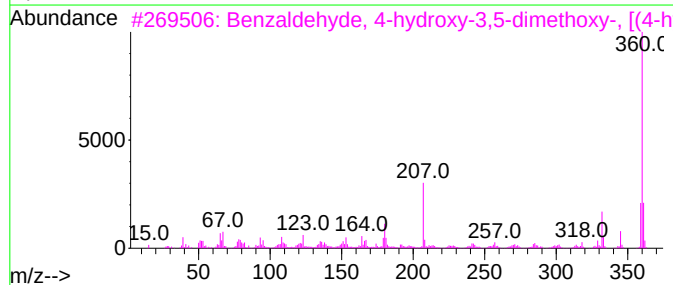
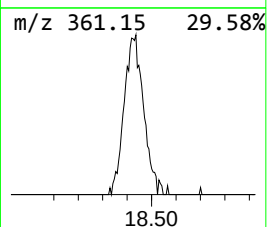
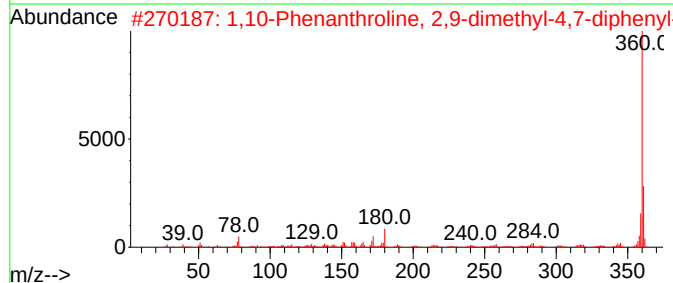
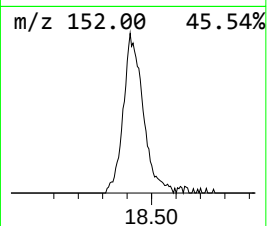
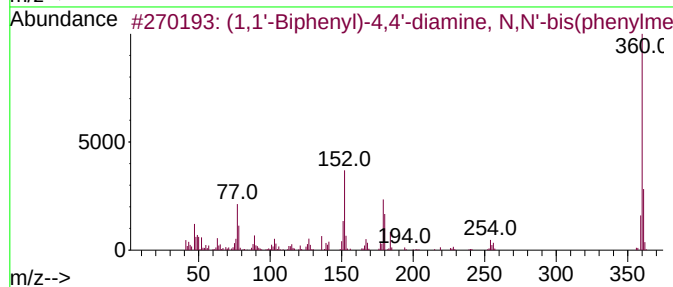
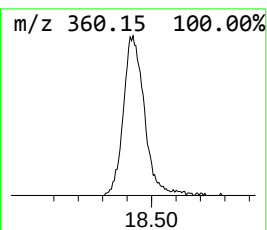
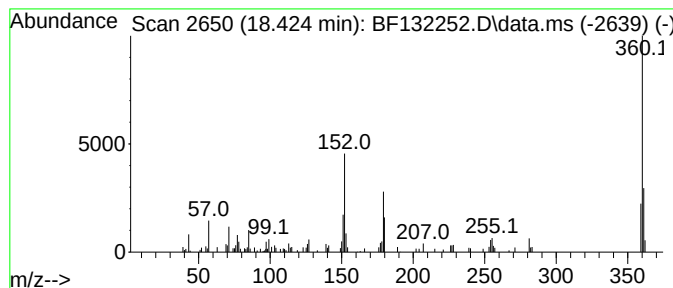
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Peak Number 4 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.424	4.59 ng	278262	Perylene-d12	15.866

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	93
2			1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	53
3			Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
4			N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	46
5			Ethene, 1-(anthracen-9-yl)-2-(4-...	360	C27H20O	1000163-55-1	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.313	35.3	ng	1760130	1	7.066	998791	20.0
Hexadecanoic ac...	13.013	2.0	ng	133337	5	14.277	1324640	20.0
Octadecanoic ac...	13.725	2.2	ng	144928	5	14.277	1324640	20.0
(1,1'-Biphenyl)...	18.424	4.6	ng	278262	6	15.866	1211550	20.0